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Comment on "Macrodispersion in Sand-Shale Sequences" by A. J. Desbarats

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1. INTRODUCTION

Desbarats [1990] used a particle-tracking scheme to investigate the physics of three-dimensional solute transport in aquifers composed of two porous media of different hydraulic conductivities. The spatially heterogeneous fluid velocity was assumed to be the only mechanism of solute movement; local or pore scale dispersion and molecular diffusion were assumed to be negligible. The particle-tracking scheme used by Desbarats consisted of routing particles from node to node in a finite difference grid. In this scheme, the direction of an individual particle is randomly selected and the probability associated with the particle movement in a given direction is proportional to the fluid flux in that direction. The same method was used by *Moreno et al.* [1988] to investigate advective transport in a variable-aperture planar fracture.

In this comment we demonstrate that the node-to-node particle-routing scheme used by Desbarats is a poor model of the physics of advective solute movement in a continuum. This scheme introduces artificial dispersion by routing particles to nodal locations on a finite difference grid, regardless of the location of fluid streamlines. Hence, the node-to-node routing scheme induces particle movement across streamlines, which is symptomatic of solute dispersion. In contrast, other particle-tracking schemes that treat a heterogeneous flow regime as a continuum and deterministically move particles based on an interpolated velocity can simulate advection-dominated solute movement without introducing artificial or numerical dispersion [e.g., *Reddell and Sunada*, 1970; *Konikow and Bredehoeft*, 1978; *Prickett et al.*, 1981].

Our comment focuses only on the errors introduced in employing the node-to-node routing scheme and its impact on interpreting advection-dominated solute movement. We do not comment on the conclusions reached by Desbarats with regard to the physics of the problem that he considered. Use of a model that accurately treats advection-dominated solute movement may or may not influence the conclusions; however, we believe that there are more appropriate and available models that can be used to investigate advection-dominated solute movement.

In the remaining sections of this comment we evaluate the artificial dispersion introduced by the node-to-node routing scheme for the case of uniform flow, and compare numerical simulations of particle movement using the node-to-node routing scheme to results of a linear velocity interpolation method for the case of a two-dimensional aquifer with binary hydraulic conductivity.

In a companion comment [*Goode and Shapiro*, this issue], we show that the node-to-node routing scheme introduces similar errors for the physical system considered by *Moreno et al.* [1988], a variable-aperture planar fracture. The results presented in this comment for the case of uniform flow apply directly to the methods used by *Moreno et al.* [1988].

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2. NODE-TO-NODE ROUTING IN UNIFORM FLOW

In a uniform flow field, with no local dispersion, an initial cloud of particles will move at the rate of the fluid velocity, with no additional spreading of the particles. The node-to-node routing scheme used by Desbarats (and by *Moreno et al.* [1988]) correctly predicts particle movement if the uniform velocity is oriented along one of the axes of the finite difference grid, because particle movement transverse to the direction of flow is given a probability of zero under such conditions. However, if the uniform velocity is not oriented with the grid, the node-to-node routing scheme artificially introduces longitudinal and transverse spreading. For flow in heterogeneous media, the local flow direction is variable, even if the mean flow direction is oriented with the grid. Hence, the node-to-node routing scheme will always introduce artificial longitudinal and transverse spreading when used to simulate transport in heterogeneous media.

The error that the node-to-node routing scheme introduces in a uniform flow field can be examined analytically. The following analysis can also be extended to three dimensions; however, for simplicity a two-dimensional finite difference grid is considered. We assume the fluid velocity to be oriented at an angle $0 \leq \theta \leq 90$, where θ is measured counterclockwise from the x axis and the finite difference grid is oriented in the x and y directions and has spatial discretization $\Delta x = \Delta y = \Delta$ (Figure 1). The components of the fluid velocity in the x and y directions are $V_x = V \cos \theta$ and $V_y = V \sin \theta$, respectively, where V is the magnitude of fluid velocity. Analytically, the time for a particle to travel a distance L in the direction of the fluid velocity is L/V.

In the node-to-node routing scheme used by Desbarats, the residence time of a particle in any block for the case of uniform flow is [after *Moreno et al.*, 1988, equation (11)]

$$t_u = \frac{\Delta}{\frac{1}{2}\sum_j |V_j|} = \frac{\Delta}{V(\cos\theta + \sin\theta)} \tag{1}$$

where t_u is the uniform residence time for all blocks, and V_j are the components of velocity from a node of interest to adjacent node j, which are computed from the finite difference interblock fluxes. The effective velocity of the particle is the distance traveled divided by the residence time. Thus, the effective velocities of particles in the node-to-node routing scheme, V_{xR} and V_{yR}, are

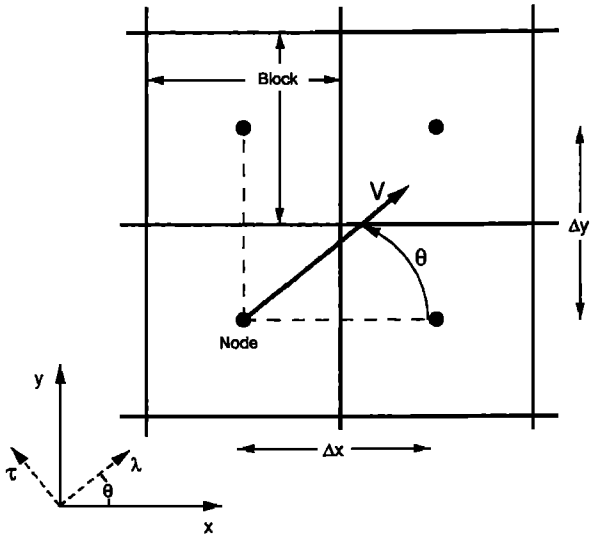

Fig. 1. Schematic of numerical grid showing spatial discretization, node-to-node connections, and orientation of velocity vector.

$$V_{xR} = V_{yR} = \frac{\Delta}{t_u} = V(\cos\theta + \sin\theta) \tag{2}$$

The node-to-node routing scheme randomly chooses either the x or y direction for each particle, but weights the probabilities of moving in a given direction by the fractional flux in either direction. For the case here, the probability of a particle moving in the positive x direction is

$$P_x = \frac{V_x}{V_x + V_y} = \frac{\cos\theta}{\cos\theta + \sin\theta} \tag{3}$$

and the probability of a particle moving in the positive y direction is

$$P_y = \frac{\sin\theta}{\cos\theta + \sin\theta} = 1 - P_x \tag{4}$$

The probabilities of particles moving in the negative x or y directions are zero because V_x and V_y are always positive for $0 \le \theta \le 90$. The expected value of the distance a particle will travel in the x direction is

$$E[L_x] = T(P_x V_{xR}) = VT\cos\theta \tag{5}$$

and the expected value of the travel distance in the y direction is

$$E[L_y] = VT\sin\theta \tag{6}$$

where T is elapsed time and $E[\ ]$ is the expected value operator. Equations (5) and (6) show that the node-to-node routing scheme preserves the mean particle position for a uniform flow field at any angle to the grid. However, because of the probabilistic method of choosing the direction of particle movement between nodes, an artificial spreading is introduced.

The longitudinal and transverse dispersion introduced by the node-to-node routing scheme in a uniform flow field can be analytically evaluated by considering the release of a large number of particles from a single node in the grid. Because the particle movement from node to node is assumed to be independent of previous particle movements, the motion of an individual particle can be regarded as a series of Bernoulli trials having one of two outcomes: (1) movement along the x direction of the grid or (2) movement along the y direction of the grid. The probability of movement in the x and y directions is given by P_x and P_y, respectively, and the binomial distribution defines the probability of the number of movements, for example, in the x direction out of the total number of particle movements. Consequently, the distance a given particle moves in the direction parallel to the uniform velocity is given by

$$L_\lambda = f\Delta\cos\theta + (N-f)\Delta\sin\theta \tag{7}$$

where L_λ is the longitudinal distance of particle movement and f is a binomially distributed random variable representing the number of times the particle has moved in the x direction out of a possible N movements. The first term on the right-hand side of (7) represents the longitudinal distance associated with particle movements in the x direction of the grid, while the second term represents the longitudinal distance associated with particle movements in the y direction of the grid. A similar expression for the location of the particle in the direction transverse to the uniform fluid velocity can also be written,

$$L_\tau = f\Delta\sin\theta - (N-f)\Delta\cos\theta \tag{8}$$

where L_τ is the transverse distance of particle movement.

Using (7) and (8), the variance of the longitudinal and transverse particle positions induced by the node-to-node routing scheme can be evaluated as

$$\sigma_\lambda^2 = E[(L_\lambda - E[L_\lambda])^2] \qquad \sigma_\tau^2 = E[(L_\tau - E[L_\tau])^2] \tag{9}$$

where σ_λ^2 and σ_τ^2 are the variances of particle location in the longitudinal and transverse directions, respectively. Effective longitudinal and transverse dispersivities (α_λ and α_τ, respectively) associated with the node-to-node routing scheme can be calculated using properties of the binomial distribution, resulting in

$$\alpha_\lambda = \frac{1}{2V}\frac{d\sigma_\lambda^2}{dt} = \frac{\Delta\sin 2\theta(1-\sin 2\theta)}{4(\cos\theta + sin\ \theta)}$$
$$\alpha_\tau = \frac{1}{2V}\frac{d\sigma_\tau^2}{dt} = \frac{\Delta\sin 2\theta(1+\sin 2\theta)}{4(\cos\theta + \sin\theta)} \tag{10}$$

Figure 2 shows the magnitude of the longitudinal and transverse dispersivities (relative to the grid spacing) that are artificially introduced by the node-to-node routing scheme in a uniform flow field as a function of the orientation of the fluid velocity. If the fluid velocity is oriented along one of the axes of the finite difference grid, the node-to-node routing scheme does not artificially introduce longitudinal or transverse dispersion into the simulations of particle movement. If, however, the fluid velocity is oriented at an angle to the finite difference grid, the node-to-node routing scheme artificially introduces both a longitudinal and transverse spreading to the particle motion, where the transverse dispersivity exceeds the longitudinal dispersivity. When flow is at 45° to the grid, the artificial transverse spreading introduced is at its maximum while the longitudinal component is zero. Both components are proportional to the grid spacing.

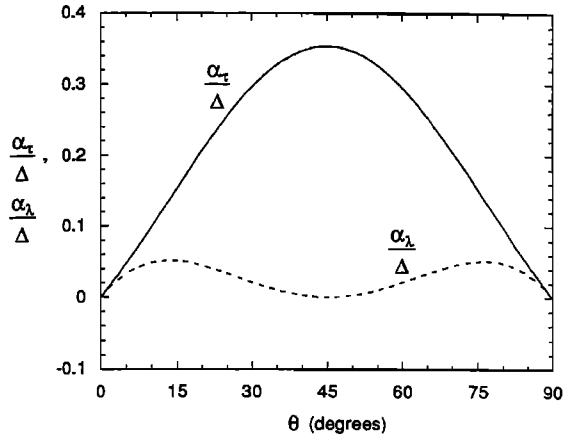

Fig. 2. Artificial dispersivities introduced by node-to-node routing in uniform flow as a function of the angle between the direction of flow and the numerical grid.

3. Node-to-Node Routing in a Binary Porous Medium

Desbarats considered three-dimensional flow of an incompressible fluid in heterogeneous porous media and applied a standard block-centered seven-point finite difference method with harmonic mean interblock hydraulic conductivity (K). Desbarats considered the hydraulic conductivity of each finite difference block to be a random indicator function taking on only two values corresponding to shale and sandstone. The indicator random function allowed the specification of the proportion of shale to sandstone, and of the spatial correlation structure in K. Also, the contrast in the conductivities of the shale and sandstone was varied from no contrast (homogeneous media) to the sandstone K being 10,000 times the shale value.

Desbarats used the node-to-node routing scheme to simulate transport through the binary heterogeneous medium. Desbarats erroneously stated that conventional particle tracking will not work for his case, but presents no analyses supporting this claim. Desbarats stated (p. 155),

> Models based on the covection-dispersion equation [*Konikow and Bredehoeft*, 1978] are adversely affected by numerical dispersion due to the convective solute flux term and are unusable here. Particle tracking models [*Ahlstrom et al.*, 1977; *Prickett et al.*, 1981] are also judged unsuitable in the present context .... These interpolated velocities are smoothed considerably and no longer reflect the true variability of the discrete velocity field. ... Finally, with high conductivity contrasts, a very small time step must be used for particle advancement. This slows computation ...

Several misrepresentations in these statements are discussed in turn.

Desbarats is probably aware that the cause of numerical dispersion lies in the numerical solution of the advection-dispersion equation by finite difference and finite element methods, not in the equation itself. The model of *Konikow and Bredehoeft* [1978] uses the method of characteristics (MOC) instead of finite differences or finite elements to simulate advection specifically because the MOC does not introduce numerical dispersion when the dispersion coefficients are zero. *Garabedian and Konikow* [1983] developed a version of the model of *Konikow and Bredehoeft* [1978] to track sharp fronts with no dispersion, numerical or physical. *Goode* [1990] demonstrates the ability of particle-tracking models using velocity interpolation to handle highly variable velocities, and *Pollock* [1988] presents a three-dimensional interpolation scheme that has been applied without difficulty to systems with large K contrasts. These investigators show that the linear interpolation of velocities (or fluxes) satisfies the fluid continuity equation within each block of the model. That is, the smooth nature of the velocity variability within each block is a result of the physics of the problem. *Goode* [1987, 1990] specifically addresses the discontinuities in V that occur where K changes abruptly; linear interpolation of velocity (and other possible schemes) preserves this physical effect. The node-to-node routing scheme actually yields a smoother breakthrough curve than linear velocity interpolation [*Goode and Shapiro*, this issue], due to the former's artificial dispersion. No artificial dispersion is introduced in velocity interpolation schemes because the particles are advected through the continuous domain without mixing at nodes, and particles do not cross streamlines.

Finally, for the case of linear interpolation of V, the path line and travel time within each block can be evaluated analytically [*Pollock*, 1988; *Goode*, 1990] and are insensitive to time step size. Only one step is required for each block, as in Desbarats' scheme. Here, we use linear interpolation with analytical evaluation of pathlines within each block. This model worked without difficulty for cases of K contrasts of up to 10,000 to 1. As for computational effort, our limited experience indicates that interpolation is of the same order of computational burden as the node-to-node routing scheme and both are certainly within the capabilities of modern computers.

Numerous investigators have applied particle-tracking schemes with velocity interpolation to study solute transport in heterogeneous media and resultant macrodispersion [e.g., *Smith and Schwartz*, 1980; *Davis*, 1986; *El-Kadi*, 1988]. Linear and other velocity interpolation methods treat the flow system as a continuum and move particles throughout the domain by computing the velocity at any point in the domain. Each separate particle follows a unique deterministic path corresponding to a streamline in steady flow. These methods have been used extensively to simulate advection in groundwater flow systems [e.g., *Reddell and Sunada*, 1970; *Konikow and Bredehoeft*, 1978; *Prickett et al.*, 1981]. The linear velocity interpolation method yields exact solutions for advection-only transport in the uniform flow case discussed above, regardless of orientation of the grid.

Schwartz [1977] used particle tracking and velocity interpolation to analyze transport in binary porous media for K contrasts of up to 83 to 1. In fact, Desbarats' conclusions that a Fickian model of macroscopic dispersion is not applicable, and that macroscopic dispersion is controlled by the magnitude of K contrasts, by the relative proportions of the two media, and by the spatial structure of the aquifer, have all previously been presented by *Schwartz* [1977].

To illustrate the differences between the node-to-node routing scheme used by Desbarats and linear velocity interpolation as used by numerous other investigators, we present results from an example simulation in a two-dimensional binary heterogeneous aquifer with sandstone and shale conductivities of 10 and 0.001 m/d, a contrast of 10,000 to 1. Using the turning bands method [*Mantoglou and Wilson*, 1982; *Zimmerman and Wilson*, 1989], we generate a normally distributed ($N[0, 1]$) random field for a grid of 51 (x)

by 31 (y) blocks having $\Delta x = \Delta y = 1$ m. The random variable is assumed to have a negative exponential and isotropic covariance function

$$R(r) = \exp\left(\frac{-|r|}{\Lambda}\right) \tag{11}$$

where R is the covariance, r is the separation distance, and the correlation length, $\Lambda = 5$ m. To convert this to an indicator function, we vary the indicator cutoff (Desbarats' y, p. 154) until the desired proportion of sandstone and shale is achieved. For the simulations presented here, the aquifer is approximately 70% sandstone. Note that we have not attempted to match the covariance structure of Desbarats' indicator K function, in part because the actual correlation function of the underlying normal random variable (his $\rho_y(h)$, p. 154) used by Desbarats was not presented. However, this K field is qualitatively similar to the correlated isotropic fields used by Desbarats and exhibits spatial correlation significantly larger than the grid blocks.

Advective transport through a single realization of the heterogeneous porous medium is performed for 1000 particles using both an implementation of Desbarats' node-to-node routing scheme and linear velocity interpolation. No-flow boundary conditions are imposed on the top ($y = 31$ m) and bottom ($y = 0$ m) borders of the grid. Fixed head boundaries are applied at nodes along the left ($x = 0.5$ m) and right ($x = 50.5$ m) borders to yield a mean velocity in the positive x direction. Particles are injected on the inflow face in proportion to the flux in the x direction at each block. For the node-to-node routing scheme, all of the particles in a given block originate at the node. In the case of velocity interpolation, the particles in a given block are initially evenly spaced in the vertical (y) direction within the block. Figure 3*a* shows the locations of all particles using the node-to-node routing scheme after 0.5 days. The number of particles in each subregion is represented by the number of petals on the "flower." A single point indicates only one particle in the subregion. Figure 3*b* shows the locations of all particles at 0.5 days using linear velocity interpolation. Although there are many similarities between the results of the two methods, such as lower velocity in the lower left part of the figures and higher density of particles in high-flow channels, the artificial dispersion introduced using the node-to-node routing scheme is readily apparent. Simulation with additional particles would increase the resolution of the front using velocity interpolation.

Differences in particle breakthrough predicted by the two approaches for the case of a binary porous medium are similar to the differences presented in a companion comment [*Goode and Shapiro*, this issue] for the case of a variable-aperture planar fracture. The residence times of most particles are overestimated and the breakthrough curve is smoother when the node-to-node routing scheme is used. There is variability in the residence times of the slowest particles using the routing scheme due to its probabilistic approach. For most node-to-node routing simulations (changing only the seed for the random number generator) on this flow field, the slowest particle had a shorter residence time than that using linear velocity interpolation.

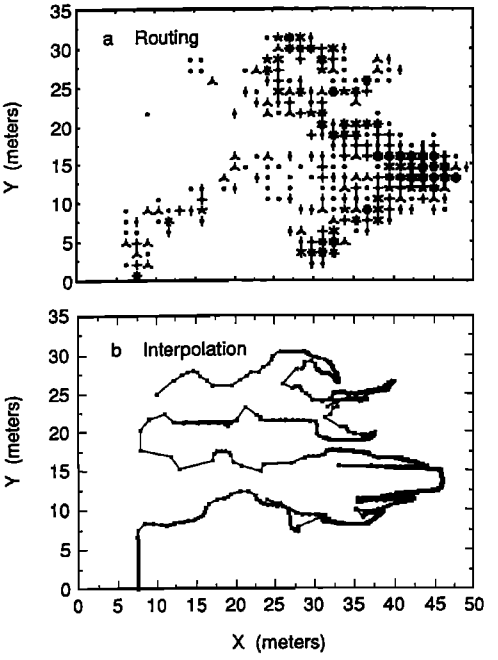

Fig. 3. Positions of 1000 particles in a binary porous medium at 0.5 days using (*a*) node-to-node routing and (*b*) velocity interpolation. In Figure 3*a* the number of particles in each subregion is indicated by the number of petals on the "flower." A single point indicates only one particle in the subregion.

4. CONCLUSIONS

Many investigators have used numerical simulations of solute transport in subsurface environments to analyze the effects of spatial variability in formation properties. This approach to the investigation of the physics of solute movement is appealing because the investigator has complete control and perfect knowledge of the formation properties. However, these numerical experiments substitute for reality only to the extent that the underlying models of flow and transport capture the physics of these processes in real systems.

Desbarats investigated solute movement in heterogeneous subsurface environments in which advection was considered to be the only process affecting transport. However, his numerical model introduced artificial dispersion into the simulations. The errors introduced using the node-to-node routing scheme were analytically calculated for a uniform flow field. In addition, we illustrated these errors in a binary heterogeneous porous media by considering numerical experiments similar to those presented by Desbarats. In this comment, we did not analyze the physical interpretations of the numerical model result. However, other particle-tracking methods that do not introduce artificial dispersion are available and are of the same order of computational burden as the node-to-node routing scheme. We hope that this discussion will contribute to the use of appropriate methods for simulation of advection transport in heterogeneous flow regimes.

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